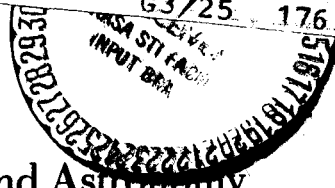


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Statistical Mechanics of  
"Negative Temperature" States

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## ABSTRACT

The dynamics of two-dimensional interacting "line" vortices is identical to that of the two-dimensional electrostatic guiding center plasma. Both are Hamiltonian systems and are therefore susceptible to statistical mechanical treatments. The predictions of the microcanonical ensemble are explored for this system. Interest focuses primarily on the regime of total positive interaction energy, which should be above the Onsager "negative temperature" threshold. Calculations of the probability distribution for a component by means of the central limit theorem are carried out in the manner of Khinchin. The probability distribution of a component reduces to the usual Gibbs distribution in the regime of positive temperatures, and is still explicitly calculable for negative temperatures. The negative temperature states are neither quiescent nor spatially uniform. Expressions for the temperature are explicitly provided in terms of the total particle energy and particle number. An extensive "thermodynamic limit" appears not to exist for the system. A BBGKY hierarchy can be derived for both temperature regimes. A Vlasov approximation on the first pair of BBGKY equations leads to the differential equation (two dimensions)  $\nabla^2 \Psi + \sinh \Psi = 0$ . The charge (vortex) density has an expectation value proportional to  $\nabla^2 \Psi$ . Numerical simulations involving solutions of the equations of motion of 4008 particles are presented.

## I. INTRODUCTION

In 1949, Onsager made what was apparently the first application of statistical mechanics to a number of interacting discrete "line" vortices.<sup>1</sup> He observed that the finiteness of the total phase space available had peculiar implications, if one attempted to apply the standard equilibrium formulas. In particular, above certain values of the total interaction energy (a constant of the motion), the thermodynamic temperature was observed to be formally negative.<sup>2</sup>

Discrete line vortices as a model for two-dimensional hydrodynamic flows then received relatively little attention for the following twenty years. Two-dimensional continuum models of hydrodynamic turbulence, in particular the two-dimensional Navier-Stokes equation, occupied the attention of many investigators,<sup>3-10</sup> who assumed (perhaps correctly) a greater degree of realism for continuum models. Even now, the relation between discrete and continuous models of two-dimensional hydrodynamic fluids remains unclear. But the subject matter of this article is primarily the discrete vortex model of Onsager<sup>1</sup> (see also Lin<sup>11</sup>).

The dynamics of the Onsager model has recently been shown to be identical to that of a two-dimensional guiding-center plasma. In this model,<sup>12</sup> very long electrostatically interacting rods remain aligned parallel to an external magnetic field and move across it with the

self-consistent  $\vec{E} \times \vec{B}$  drift. This model has been the point of origin for a number of analytical and/or numerical calculations.<sup>12-20</sup> It is not our purpose to give a general review or assessment of these here.

We shall be concerned primarily with a semi-rigorous application of the methods of equilibrium statistical mechanics to the guiding center plasma (or equivalently, the line vortex system). An earlier paper<sup>21</sup> presented numerical simulations of the motions of the system and obtained some of the present results heuristically.

Specifically, we are concerned with adapting the apparatus of the theory of probability in the form given by Khinchin<sup>22</sup> to obtain ensemble-average predictions for the states of the guiding center plasma at arbitrary values of the ratio of the total interaction energy to total particle number. We anticipate that above certain values of this ratio,<sup>1</sup> macroscopically stationary and spatially uniform thermodynamic equilibria do not exist.<sup>2,17</sup> The novel point is that, nevertheless, predictions can be extracted concerning the nature of the macroscopic states. It should be remarked that an understanding of the material in Chaps. 2, 4, and 5 of Khinchin<sup>22</sup> is mandatory for a satisfactory understanding of the present paper.

Section II details the dynamics of the model. Section III formulates the problem in the language of the theory of probability. Section IV applies the central limit theorem to calculate the analogue of the usual Gibbs distribution for the guiding center plasma, though

the content of the result is radically different. Section V derives an analogue of the BBGKY hierarchy which applies to negative temperature states. Section V also treats the hierarchy in the "Vlasov limit," leading to a nonlinear partial differential equation which we believe to be of central importance in the subject. Section VI illustrates the results with a numerical simulation of the system.

## II. EQUATIONS OF MOTION

The equations of motion of the line vortex system are

$$\frac{d\vec{x}_i}{dt} = \sum_{j \neq i} \frac{\vec{K}_j}{2\pi} \times \frac{\vec{x}_{ij}}{x_{ij}^2} \quad (1)$$

where  $\vec{x}_i = (x_i, y_i)$  is the two-component vector which locates the  $i$ th vortex of strength  $\vec{K}_i = K_i \hat{e}_z$ .  $\vec{x}_{ij} \equiv \vec{x}_i - \vec{x}_j$ . Eqs. (1) also represent the equations of motion of the two-dimensional guiding-center plasma, if we make the replacement

$$\vec{K}_j = - \frac{4\pi c e_j \vec{B}}{\ell B^2}, \quad (2)$$

where  $\vec{B}$  is a uniform magnetic field  $\vec{B} = B \hat{e}_z$ ,  $c$  is the speed of light,  $e_j$  is the charge on the  $j$ th rod, and the rods, all aligned parallel to the  $z$ -axis, have a very long length  $\ell$ . We are thus free to discuss the two systems interchangeably. In most of our discussion, we shall use the plasma vocabulary.

Eq. (1) can be given a Hamiltonian form by defining canonical coordinates

$$(q_j, p_j) = \left| K_j \right|^{\frac{1}{2}} (x_j, y_j \text{ sgn } K_j) \quad (3)$$

and Hamiltonian function

$$H = - (2\pi)^{-1} \sum_{i < j} K_i K_j \ln |\vec{x}_{ij}| \quad . \quad (4)$$

Hamilton's equations

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = - \frac{\partial H}{\partial q_i} \quad (5)$$

then reproduce Eqs. (1). Since  $H$  is not explicitly a function of time, it is a constant of the motion for an isolated system. It is convenient to work with the total Coulomb interaction energy, which is proportional to  $H$ :

$$\mathcal{E} = \sum_{i < j} \varphi_{ij} = - 2 \sum_{i < j} \frac{e_i e_j}{l} \ln |\vec{x}_{ij}| \quad . \quad (6)$$

The sum runs over all pairs of charges. Hereafter, we shall assume there are  $N$  of  $+e$  and  $N$  more of  $-e$  in a large volume  $V = L^2$ .

It will be convenient for later purposes to expand the electric field due to the  $j$ th charge (say) in a Fourier series, assuming periodic boundary conditions over a box of large volume  $V = L^2$ :



$$\vec{E}(\vec{x};\vec{x}_j) = - \sum_{\vec{k}} \frac{4\pi i k e_j}{k^2 \ell V} \exp i\vec{k} \cdot (\vec{x} - \vec{x}_j) \quad , \quad (7)$$

and the total electric field due to all charges is

$$\vec{E}(\vec{x}) = \sum_j \vec{E}(\vec{x};\vec{x}_j) \quad . \quad (8)$$

The integral  $\ell \int_V \vec{E}^2(\vec{x}) d\vec{x} / 8\pi$  can be interpreted as the total energy  $\mathcal{E}$  if we remember to subtract off the Coulomb self-energy of each charge. This is the total number of charges times

$$\ell \int_V (\vec{E}(\vec{x};\vec{x}_j))^2 \frac{d\vec{x}}{8\pi} = \frac{2\pi e^2}{\ell V} \sum_{\vec{k}} 1/k^2 \quad . \quad (9)$$

The total Coulomb self-energy of all  $2N$  charges ( $N$  of the  $+e$  and  $N$  more of  $-e$ ) is, therefore,

$$\mathcal{E}_{\text{self}} \equiv \frac{4\pi N e^2}{\ell V} \sum_{\vec{k}} 1/k^2 \quad .$$

It may be useful for some purposes to render  $\mathcal{E}_{\text{self}}$  finite by cutting off the  $\sum_{\vec{k}}$  at  $|\vec{k}| = k_{\text{max.}}$ , say, where  $k_{\text{max.}}$  is some maximum wave number the reciprocal of which is much less than the mean interparticle

spacing  $[L^2/2N]^{\frac{1}{2}}$ . The minimum value of  $\vec{k}$  in Eq. (9) is, of course,  $2\pi/L$ . The complete expression for the interaction energy  $\mathcal{E}$  is, then, alternatively written as Eq. (6) or

$$\begin{aligned}\mathcal{E} &= \ell \int_V d\vec{x} \frac{\vec{E}^2(\vec{x})}{8\pi} - \mathcal{E}_{\text{self}} \\ &= \frac{2\pi}{\ell V} \sum_{\vec{k}} \sum_{i,j} \frac{e_i e_j}{k^2} \exp i\vec{k} \cdot (\vec{x}_i - \vec{x}_j) - \frac{4\pi N e^2}{\ell V} \sum_{\vec{k}} 1/k^2 \\ &= \frac{2\pi}{\ell V} \sum_{\vec{k}} \sum_{i \neq j} \frac{e_i e_j}{k^2} \exp i\vec{k} \cdot (\vec{x}_i - \vec{x}_j) \quad , \quad (11)\end{aligned}$$

where the  $\sum_{\vec{k}}$  is again understood to be cut off at  $k_{\text{max}}$  when necessary. This should be understood as a modification of the Coulomb potential at distances much less than an interparticle spacing. It is to be hoped that the essential physics of the situation is unaffected by this modification, and we shall not inquire into the question of possible collapse of the system at large negative values of the interaction energy,<sup>23-26</sup> which might result from treating the interactions of positives and negatives without a cutoff.

### III. FORMULATION OF THE STATISTICAL PROBLEM

The equation  $\mathcal{E} = \text{const.}$  defines a surface of constant energy in the phase space of the system. A point on this surface is conveniently labelled by giving the values of the coordinates  $(\vec{x}_1, \vec{x}_2, \dots)$  for all the charges (vortices) of the system.

If the system occupies a large but finite spatial volume  $V = L^2$ , the total volume of the phase space available to  $2N$  charges varies as  $V^{2N}$ . It is the finiteness of this total available phase space which gives the system its novel features. (By contrast, the total phase space available to an ideal gas in a finite spatial volume is infinite.<sup>22</sup>)

If we define  $\Phi(\mathcal{E}_0) = \int_{\mathcal{E} < \mathcal{E}_0} d\vec{x}_1 d\vec{x}_2 \dots$  as the total volume of phase space with energy  $< \mathcal{E}_0$ , then the structure function  $\Omega(\mathcal{E}_0)$ ,

$$\Omega(\mathcal{E}_0) \equiv \Phi'(\mathcal{E}_0) = \int d\vec{x}_1 d\vec{x}_2 \dots \delta(\mathcal{E}_0 - \mathcal{E})$$

will necessarily pass through a maximum (at  $\mathcal{E} = \mathcal{E}_m$ , say) as  $\mathcal{E}_0$  increases. The familiar classical formulas for the entropy and temperature,

$$S = \kappa \ln \Omega(\varepsilon_0) + \text{const.},$$

$$(\kappa T)^{-1} = \Omega'(\varepsilon_0)/\Omega(\varepsilon_0) \quad ,$$

will predict formally that when  $\varepsilon_0 > \varepsilon_m$ , the temperature  $T$  will be negative.<sup>1,2</sup> ( $\kappa$  is Boltzmann's constant.)

In this article, we are mainly concerned with the following question. If one makes the hypothesis of equal a priori probabilities, and assumes a uniform probability distribution for the phase space variables  $\vec{x}_1, \vec{x}_2, \dots$  over the energy shell at  $\varepsilon = \varepsilon_0$ , what is the probability distribution law for a small component of the system in its own space?

This is the question the answer to which in the classical cases<sup>22</sup> leads to the Gibbs distribution: the well-known derivation of the canonical ensemble from the microcanonical ensemble. For  $\varepsilon_0 < \varepsilon_m$ , we may also expect a Gibbs distribution to result. The more interesting question is, What will result when  $\varepsilon_0 > \varepsilon_m$ ?

Components are defined technically as groups of charges which interact only weakly with charges in other groups.<sup>22</sup> That is, the total energy  $\varepsilon$  can be written to a good approximation as

$$\varepsilon \approx \varepsilon_1 + \varepsilon_2 + \dots + \varepsilon_n \quad (12)$$

in a case where there are  $n$  components.  $\varepsilon_k$  is the sum of the pairwise potential energies for all the charges in the  $k$ th component. The

microcanonical ensemble can then be defined for a system which is idealized as consisting of  $n$  large spatial volumes containing many charges each, but spatially well separated so that the charges in each volume interact strongly only among themselves.

The random vector  $\vec{x}_1, \vec{x}_2, \dots$  is then assigned a probability distribution

$$\begin{aligned} P(\vec{x}_1, \vec{x}_2, \dots) &= \frac{\delta(\mathcal{E}_0 - \mathcal{E})}{\int d\vec{x}_1 d\vec{x}_2 \dots \delta(\mathcal{E}_0 - \mathcal{E})} \\ &= \frac{\delta(\mathcal{E}_0 - \mathcal{E})}{\Omega(\mathcal{E}_0)} \end{aligned} \quad (13)$$

It is shown by Khinchin,<sup>22</sup> and the proof can be readily adapted for this system, that the combination law for the structure functions of  $n$  components is

$$\Omega(\mathcal{E}_0) = \int \left( \prod_{k=1}^{n-1} \Omega_k(\mathcal{E}_k) d\mathcal{E}_k \right) \Omega_n \left( \mathcal{E}_0 - \sum_{k=1}^{n-1} \mathcal{E}_k \right) \quad (14)$$

Here  $\Omega_k$  is the structure function for component  $k$  of energy  $\mathcal{E}_k$ .

Any sum of components satisfying Eq. (12) is also a component. If the total system is divided into just two components, the probability distribution law for component 1 (say) in its own phase space is<sup>22</sup>

$$P(1) = \Omega_2(\varepsilon_0 - \varepsilon_1)/\Omega(\varepsilon_0) \quad . \quad (15)$$

The main computational problem we have is in evaluating asymptotic forms for the terms in Eq. (15), and this is addressed in the next section.

## IV. APPLICATION OF THE CENTRAL LIMIT THEOREM

The structure function  $\Omega(\epsilon)$  for our system is normalizable, in the sense that its moments can be assumed to exist. Random-phase estimates of the first few of these are derived in the Appendix.  $\Omega(\epsilon_0)$  is non-negative and obeys the combination law (14), and so may be treated formally as a probability distribution law for a sum of uncorrelated random quantities  $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ , upon dividing each  $\Omega_k$  by  $V^{2N_k}$ .  $2N_k$  is the total number of charges in the kth component.  $2N = \sum_k 2N_k$  is the total number of charges in all components.

It is important to realize that not much physical significance attaches to the probability distribution laws  $\Omega_k/V^{2N_k}$  and  $\Omega(\epsilon_0)/V^{\sum_k 2N_k} = \Omega(\epsilon_0)/V^{2N}$  directly. The physically significant distribution laws are Eqs. (13) and (15). Treating

$$\frac{\Omega(\epsilon_0)}{V^{2N}} = \frac{\Omega(\epsilon_1 + \epsilon_2 + \dots + \epsilon_n)}{V^{2N}} \text{ as the probability distribution law}$$

of a large number  $n$  of uncorrelated random variables is mainly a mathematical convenience. This convenience lies in the applicability of the central limit theorem from the theory of probability,<sup>22</sup> which enables one to write down asymptotic distribution laws for such sums as the number  $n$  of terms in the sum becomes large compared to unity. These asymptotic forms can then be used to evaluate Eq. (15).

Since our  $\Omega_k$ 's are normalizable, our task is in some respects simpler than Khinchin's. It is the lack of normalizability of  $\Omega_k$ 's for systems having a classical unbounded momentum space which necessitates<sup>22</sup> introduction of the "generating functions" and normalizable "conjugate distribution laws" to which the central limit theorem can be applied. We need not make this detour, but can apply the central limit theorem directly to the  $\Omega_k/V^{2N_k}$ .

The essential content of the central limit theorem<sup>22</sup> is that for relatively mild restrictions on the  $\Omega_k(\epsilon_k)$ ,

$$\frac{\Omega(\epsilon_0)}{V^{2N}} \xrightarrow{n \rightarrow \infty} \frac{\exp\{-(\epsilon_0 - A_n)^2/2B_n\}}{(2\pi B_n)^{\frac{1}{2}}} \quad (16)$$

up to terms of  $O(n^{-1})$ .  $2N$  is the total number of particles in all the components:  $2N = \sum_k 2N_k$ .  $A_n$  is defined by

$$A_n = \sum_{k=1}^n a_k = \sum_{k=1}^n \int \epsilon_k \frac{\Omega_k(\epsilon_k) d\epsilon_k}{V^{2N_k}}$$

and is the sum of the expectations of the first  $n$  random quantities.

$B_n$  is defined by

$$B_n = \sum_{k=1}^n b_k = \sum_{k=1}^n \int (\epsilon_k - a_k)^2 \frac{\Omega_k(\epsilon_k) d\epsilon_k}{V^{2N_k}}$$



and is the sum of their dispersions. This result is independent of the detailed nature of the  $\Omega_k$ .

In the Appendix, expressions for  $a_k$  and  $b_k$  are derived within the framework of the random phase approximation. It is shown there that  $a_k = 0$ , and (see Eq. (A-10))  $b_k = (N_k e^2 / \ell)^2 / \pi$ , where  $2N_k$  is the total number of charges in the  $k$ th component. The expression (16) then implies that up to terms of  $O(1/n)$ ,

$$\frac{\Omega(\epsilon_0)}{V^{2N}} = \frac{\exp\{-\epsilon_0^2 / 2 \sum_k b_k\}}{\sqrt{2\pi \sum_k b_k}} \quad (17)$$

In the evaluation of formula (15), we treat component 1 as a finite system, with number of degrees of freedom and total energy as of  $O(1)$ . We treat both component two (all the rest of the total system) and the total system as very large, with number of components and total energy as of  $O(n)$ ,  $n \gg 1$ . The sums  $\sum_{k=1}^n b_k$  and  $\sum_{k=2}^n b_k$  are both  $O(n)$  quantities which differ only by terms of  $O(1)$ , so their difference can be neglected. We find from Eq. (15) that

$$\left( B \equiv \sum_{k=1}^n b_k = O(n) \right)$$

$$P(1) = \frac{1}{V^{2N_1}} \frac{\exp\{-(\epsilon_0 - \epsilon_1)^2 / 2B\}}{\exp\{-\epsilon_0^2 / 2B\}} \quad (18)$$

As long as  $\epsilon_1 \ll \epsilon_0$ , Eq. (18) reduces to

$$P(1) = \frac{1}{2N_1} \exp\{\epsilon_0 \epsilon_1 / B\} \quad . \quad (19)$$

When  $\epsilon_0/B$ , which is proportional to the total interaction energy, is negative, Eq. (19) is the canonical distribution of Gibbs, with positive "temperature"  $(kT)^{-1} = -\epsilon_0/B$ . The explicit value of  $B$  is

$$B = \sum_{\text{(components)} k} (N_k e^2 / \ell)^2 / \pi \quad ,$$

where  $2N_k$  is the total number of charges in the  $k$ th component.

For  $\epsilon_0 > 0$ , the canonical ensemble again formally appears, but the "temperature",  $-B/\epsilon_0$ , is negative.  $P(1)$  is still normalizable, however, because of the decay of  $\Omega_1(\epsilon_1)$  at large  $\epsilon_1$ , for all values of  $\epsilon_0$ . It is meaningful to inquire into the values of ensemble averages computed with the probability distributions (18) or (19) just as it is for the more conventional Gibbs distribution. It should come as no surprise that some of the ensemble averaged quantities have different qualitative features than they do in the positive-temperature case, however.

We note in passing that Taylor's<sup>18</sup> random phase result,  $\epsilon_m = 0$ , (corrected for the Coulomb self-energy) has been confirmed by Eq. (19).

The random phase approximation has been used in the Appendix to provide a specific numerical value for  $B$ , and to show that the  $a_k = 0$ .

The canonical distribution law of a component, Eq. (19), with  $\epsilon_0/B > 0$ , apparently does not imply an extensive thermodynamic limit for the component in the conventional sense.<sup>20</sup> For the expectation value of the energy of component 1, given by using Eq. (19) in  $\int d\epsilon_1 P(1)\Omega_1(\epsilon_1)\epsilon_1 / \int d\epsilon_1 P(1)\Omega_1(\epsilon_1)$ , can be shown via the random phase approximation to vary proportionally to  $N_1^2$  rather than  $N_1$ , at least for small, fixed  $\epsilon_0/B$ . ( $2N_1$  is the number of charges in component 1.) This emphasizes the necessity of rethinking from the beginning any macroscopic thermodynamic concepts one may wish to apply to this model. Variables such as the total energy are not extensive in the usual thermodynamic sense.

## V. BBGKY HIERARCHY

The canonical distribution (19) can be used as the basis for a BBGKY hierarchy even though  $\epsilon_0/B$  may be positive. Define the probability distribution of the first  $s_i$  positive charges and  $s_e$  negative charges by, as usual,<sup>13,20</sup>

$$n_{s_i, s_e} = V^{s_i + s_e} \int d\vec{x}_{s_i+1}^i \dots d\vec{x}_{N_1}^i d\vec{x}_{s_e+1}^e \dots d\vec{x}_{N_1}^e P(1) \quad (20)$$

Here,  $\vec{x}_\ell^i$  is the vector position of the  $\ell$ th "ion", and  $\vec{x}_\ell^e$  that of the  $\ell$ th "electron".  $P(1)$  is given by Eq. (19). Setting  $\theta \equiv -B/\epsilon_0$ ,

$$\begin{aligned} & \frac{\partial n_{s_i, s_e}}{\partial \vec{x}_j^e} + \frac{n_{s_i, s_e}}{\theta} \frac{\partial \Phi(s_i, s_e)}{\partial \vec{x}_j^e} \\ &= - \frac{n_0}{\theta} \int d\vec{x}_{s_i+1}^i \frac{\partial \varphi^{ei}(\vec{x}_j^e - \vec{x}_{s_i+1}^i)}{\partial \vec{x}_j^e} n_{s_i+1, s_e} \\ & \quad - \frac{n_0}{\theta} \int d\vec{x}_{s_e+1}^e \frac{\partial \varphi^{ee}(\vec{x}_j^e - \vec{x}_{s_e+1}^e)}{\partial \vec{x}_j^e} n_{s_i, s_e+1} \quad (21) \end{aligned}$$

Here  $j$  is any number between 1 and  $s_e$ , and  $n_o = N_1/V$ .

$\varphi^{ii} = \varphi^{ee} = -\varphi^{ei} = -\varphi^{ie}$  is the two-body Coulomb interaction of

Eq. (6).  $\Phi(s_i, s_e)$  is the sum of the pairwise Coulomb interactions

among the first  $s_i$  ions and the first  $s_e$  electrons. A similar hierarchy can be obtained by taking gradients with respect to ion coordinates.

The hierarchy (21) is identical with the conventional hierarchy<sup>20</sup> except that  $\theta$  may be negative, and is so in the case of most interest.

For negative temperatures, Eqs. (21) will not be tractable by the usual methods. We do not expect  $n_{1,o}$  and  $n_{o,1}$  to be spatially uniform for  $\theta < 0$ . It is interesting to try a "Vlasov approximation" on (21), approximating  $n_{2,o} \approx n_{1,o} n_{1,o}$ ,  $n_{o,2} \approx n_{o,1} n_{o,1}$ , and  $n_{1,1} \approx n_{1,o} n_{o,1}$ . The result is

$$\begin{aligned}
 \frac{\partial n_{o,1}}{\partial \vec{x}_1^e} &= -\frac{n_o}{\theta} \int d\vec{x}_1^i \frac{\partial \varphi^{ei}(\vec{x}_1^e - \vec{x}_1^i)}{\partial \vec{x}_1^e} n_{1,o}(\vec{x}_1^i) n_{o,1}(\vec{x}_1^e) \\
 &\quad - \frac{n_o}{\theta} \int d\vec{x}_2^e \frac{\partial \varphi^{ee}(\vec{x}_1^e - \vec{x}_2^e)}{\partial \vec{x}_1^e} n_{o,1}(\vec{x}_1^e) n_{o,1}(\vec{x}_2^e) \\
 \frac{\partial n_{1,o}}{\partial \vec{x}_1^i} &= -\frac{n_o}{\theta} \int d\vec{x}_1^e \frac{\partial \varphi^{ei}(\vec{x}_1^i - \vec{x}_1^e)}{\partial \vec{x}_1^i} n_{1,o}(\vec{x}_1^i) n_{o,1}(\vec{x}_1^e) \\
 &\quad - \frac{n_o}{\theta} \int d\vec{x}_2^i \frac{\partial \varphi^{ii}(\vec{x}_1^i - \vec{x}_2^i)}{\partial \vec{x}_1^i} n_{1,o}(\vec{x}_1^i) n_{1,o}(\vec{x}_2^i) .
 \end{aligned} \tag{22}$$

Eqs. (22) can be rewritten as

$$\begin{aligned} \frac{\partial}{\partial \vec{x}_1^e} \left\{ \ell n n_{o,1}(\vec{x}_1^e) + \frac{n_o}{\theta} \int d\vec{x}' \varphi^{ee}(\vec{x}_1^e - \vec{x}') [n_{o,1}(\vec{x}') \right. \\ \left. - n_{1,o}(\vec{x}')] \right\} = 0 \\ \frac{\partial}{\partial \vec{x}_1^i} \left\{ \ell n n_{1,o}(\vec{x}_1^i) + \frac{n_o}{\theta} \int d\vec{x}' \varphi^{ii}(\vec{x}_1^i - \vec{x}') [n_{1,o}(\vec{x}') \right. \\ \left. - n_{o,1}(\vec{x}')] \right\} = 0 \quad . \end{aligned} \quad (23)$$

Adding Eqs. (23) gives

$$\frac{\partial}{\partial \vec{x}} [\ell n n_{o,1}(\vec{x}) + \ell n n_{1,o}(\vec{x})] = 0 \quad , \quad (24)$$

or  $n_{o,1} n_{1,o} = \text{const.}$  Integrating Eqs. (23) gives

$$\begin{aligned} n_{o,1}(\vec{x}) &= c_1 \exp \left\{ \frac{n_o}{\theta} \int d\vec{x}' \varphi(\vec{x} - \vec{x}') [n_{1,o}(\vec{x}') - n_{o,1}(\vec{x}')] \right\} \\ n_{1,o}(\vec{x}) &= c_2 \exp \left\{ - \frac{n_o}{\theta} \int d\vec{x}' \varphi(\vec{x} - \vec{x}') [n_{1,o}(\vec{x}') - n_{o,1}(\vec{x}')] \right\} \quad . \end{aligned} \quad (25)$$

$c_1$  and  $c_2$  are two constants of integration satisfying  $c_1 c_2 = n_{o,1} n_{1,o}$  which are to be determined by requiring that

$$\frac{1}{V} \int n_{o,1}(\vec{x}) d\vec{x} = \frac{1}{V} \int n_{1,o}(\vec{x}) d\vec{x} = 1 \quad ; \quad (26)$$

and  $\varphi(\vec{x} - \vec{x}') = - (2e^2/\ell) \ln |\vec{x} - \vec{x}'|$  .

Defining  $\rho(\vec{x}) \equiv n_{1,o}(\vec{x}) - n_{o,1}(\vec{x})$  , Eqs. (25) can be combined to give

$$\begin{aligned} \rho(\vec{x}) = & - c_1 \exp \left\{ \frac{n_o}{\theta} \int d\vec{x}' \varphi(\vec{x} - \vec{x}') \rho(\vec{x}') \right\} \\ & + c_2 \exp \left\{ - \frac{n_o}{\theta} \int d\vec{x}' \varphi(\vec{x} - \vec{x}') \rho(\vec{x}') \right\} . \end{aligned} \quad (27)$$

On physical grounds, we expect antisymmetry of the charge distribution about the center of the box, which permits us to restrict attention to the case  $c_1 = c_2 = c$ , where

$$c = V / \int d\vec{x} \exp \left\{ \frac{n_o}{\theta} \int d\vec{x}' \varphi(\vec{x} - \vec{x}') \rho(\vec{x}') \right\} > 0 \quad . \quad (28)$$

If we then introduce a scalar potential,

$$e\Phi(\vec{x}) \equiv n_o \int \varphi(\vec{x} - \vec{x}') \rho(\vec{x}') d\vec{x}' , \text{ Eq. (27) becomes}$$

$$\nabla^2 \Phi = \frac{4\pi e n_o c}{\ell} \left[ \exp\left(\frac{e\Phi}{\theta}\right) - \exp\left(-\frac{e\Phi}{\theta}\right) \right] . \quad (29)$$

In a more compact notation, let  $\Psi \equiv e\Phi/\theta$  and  $\tilde{\nabla}^2 = \lambda_D^2 \nabla^2/c$ , with  $\lambda_D^2 \equiv \ell|\theta|/4\pi n_o e^2$ , and Eq. (29) becomes

$$\tilde{\nabla}^2 \Psi + \sinh \Psi = 0 . \quad (30)$$

The nonlinear differential equation (30) determines the charge-density distributions for the negative-temperature states. It was derived by a quite different method in Reference 21. Easily soluble in one dimension, it is apparently intractable in two, and will probably require numerical investigation. It is to be noted that if the sign of  $\theta$  were reversed, the sign of the  $\sinh \Psi$  term would be reversed in Eq. (30), leaving us with the Debye-Poisson equation in two dimensions. One effect of the negative temperature is to convert its exponentially damped linearized solutions into spatially oscillatory ones.<sup>21</sup> This set of spatially oscillatory linear solutions can be fit into the box with either perfectly-conducting or periodic boundary conditions to give density distributions qualitatively similar to those in Ref. 21, but no quantitative agreement has yet been achieved.



## VI. SIMULATION RESULTS

We do not yet know analytical ensemble average predictions for the charge densities that would follow from the solutions of Eq. (30), nor analytical estimates of the fluctuations to be expected about the ensemble average. It is perhaps instructive to present as an illustration the results of numerical simulations of the high-energy states of the system. These are expected to be a pair of macroscopic counter-rotating vortices.<sup>21,17</sup>

More details of the program by which the equations of motion of 4008 particles obeying the dynamics of Sec. II are presented elsewhere.<sup>21,27</sup> The charges are confined by a perfectly conducting boundary (for the vortex problem, the boundary is therefore a streamline) inside a rectangle of width one half the length. Loading schemes have been developed which permit arbitrary initial values to be assigned to the total energy. Most of the phase space available to the system which is consistent with very high energies corresponds to configurations in which the positive charges crowd together in one half of the box while the negatives crowd together in the opposite half. The macroscopic flow pattern this corresponds to consists of two spatially-separated counter-rotating vortices.

Shown in Fig. 1 is a plot of the fluid velocity vector at  $t = 0$  and  $t = 160$  (see Reference 21 for a discussion of the units)

for the case in which the total interaction energy for the particle-in-cell model is 2.3 times the self-energy. In Fig. 2, similar plots are given for  $t = 0$  and  $t = 375$  for an interaction energy 0.43 times the self-energy. The degree to which the macroscopic counter-rotating vortices form and the speed with which they form both qualitatively increase as the interaction energy increases. The capacity of such plots as Figs. 1 and 2 to display any such macroscopic ordering as the interaction is decreased disappears before the threshold (zero interaction energy) is reached. But it has been noted elsewhere<sup>21</sup> that spectral density plots of  $\left| \vec{E}(k_x, k_y) \right|^2$  do show qualitative differences above and below zero interaction energy.

APPENDIX: RANDOM PHASE APPROXIMATION TO  $\Omega(\varepsilon_0)$ 

In this Appendix, we elaborate and extend Taylor's approximate<sup>18</sup> calculation of

$$\Omega(\varepsilon_0) = \int d\vec{x}_1 d\vec{x}_2 \dots \delta(\varepsilon_0 - \varepsilon) \quad (\text{A-1})$$

where  $\varepsilon$  is given by Eq. (10). In addition, we are interested in determining the moments of  $\Omega(\varepsilon_0)$  and the character of its approach to zero at large  $\varepsilon_0$ .

The essence of the random phase approximation as applied to this problem is the introduction of the variables  $r_{\vec{k}}$ ,

$$\rho_{\vec{k}} = \sum_j \frac{e_j}{\ell V} \exp(-i\vec{k} \cdot \vec{x}_j) = r_{\vec{k}} \exp(i\varphi_{\vec{k}}) \quad (\text{A-2})$$

as independent variables in place of the particle coordinates  $\vec{x}_j$ .

It is assumed that convergence can be achieved by taking the number independent  $\vec{k}$ 's as equal to the number of degrees of freedom (in this case  $4N$ ) and taking both very large. This large number can be identified with the number of  $\vec{k}$ 's in the sums of Sec. II. The random phase approximation to the energy amounts to a neglect of terms with  $\vec{k} + \vec{k}' \neq 0$  in the double sum

$$\vec{E}^2 = - \sum_{\vec{k}, \vec{k}'} \frac{16\pi^2 \vec{k} \cdot \vec{k}'}{k^2 k'^2} \rho_{\vec{k}} \rho_{\vec{k}'} \quad (A-3)$$

This reduces  $\vec{E}^2$  to the random phase expression

$$\vec{E}^2 \approx 16\pi^2 \sum_{\vec{k}} r_{\vec{k}}^2 / k^2 \quad (A-4)$$

independently of the values of the phases  $\varphi_{\vec{k}}$ .

It is then possible to show that the transformation

$$(\vec{x}_1, \vec{x}_2, \dots) \rightarrow \left( r_{\vec{k}_1}^2, r_{\vec{k}_2}^2, \dots \right)$$

has the Jacobian

$$J = \frac{\delta(\vec{x}_1, \vec{x}_2, \dots)}{\delta\left(r_{\vec{k}_1}^2, r_{\vec{k}_2}^2, \dots\right)} \\ = V^{2N} \prod_{\vec{k}} \left( \frac{\ell^2 V^2}{2Ne^2} \exp \left\{ - \frac{\ell^2 V^2 r_{\vec{k}}^2}{2Ne^2} \right\} \right), \quad (A-5)$$

and any integral of the form  $\int d\vec{x}_1 d\vec{x}_2 \dots$  can be converted to one

over  $\int J d\vec{r}_1^2 d\vec{r}_2^2 \dots$ , provided that the integrand depends only on the  $r_{\vec{k}}^2$ 's and not the  $\varphi_{\vec{k}}$ 's.

With these remarks, and in view of (A4) and Eq. (10), we see that we can write the expression (A1) as

$$\begin{aligned} \Omega(\mathcal{E}_0) &= \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \int d\vec{x}_1 d\vec{x}_2 \dots \exp i\lambda(\mathcal{E}_0 - \mathcal{E}) \\ &= \frac{V^{2N}}{2\pi} \int_{-\infty}^{\infty} d\lambda \int \prod_{\vec{k}} \left\{ d(r_{\vec{k}}^2) \frac{\ell^2 V^2}{2Ne^2} \exp \left[ - \frac{i\lambda 2\pi \ell V r_{\vec{k}}^2}{k^2} \right. \right. \\ &\quad \left. \left. + \frac{i\lambda 4\pi Ne^2}{\ell V k^2} - \frac{\ell^2 V^2}{2Ne^2} r_{\vec{k}}^2 \right] \right\} \exp i\lambda \mathcal{E}_0 . \end{aligned} \quad (A-6)$$

All the integrals over the  $d\vec{r}_{\vec{k}}^2$  can be done, and Eq. (A-6) can be written compactly as

$$\Omega(\mathcal{E}_0) = \frac{V^{2N}}{2\pi} \int_{-\infty}^{\infty} d\lambda \exp \left\{ i\lambda \left( \mathcal{E}_0 + \frac{4\pi Ne^2}{\ell V} \sum_{\vec{k}} \frac{1}{k^2} \right) + A(\lambda) \right\} , \quad (A-7)$$

where

$$A(\lambda) \equiv - \sum_{\vec{k}} \ell n(1 + i\alpha^2 \lambda / k^2) , \quad \alpha^2 \equiv 4\pi Ne^2 / \ell V .$$

A steepest-descent approximation to Eq. (A-7) suggests itself, since the coefficient of  $\lambda$  is, in the case of interest, a very large quantity when  $N \gg 1$ . This can be used to show that  $d\Omega(\epsilon_0)/d\epsilon_0 = 0$  when  $\epsilon_0 = 0$ . Thus the threshold for negative temperatures is  $\epsilon_0 = 0$ . (This is Taylor's result,<sup>18</sup> when the Coulomb self-energy is taken properly into account.)

Moments of the type

$$\langle \epsilon_0^m \rangle \equiv \int d\epsilon_0 \epsilon_0^m \Omega(\epsilon_0)$$

can also be evaluated by noting that

$$\begin{aligned} & \int \epsilon_0^m \Omega(\epsilon_0) d\epsilon_0 \\ &= V^{2N} \int_{-\infty}^{\infty} d\lambda (-i)^m \left( \frac{d^m}{d\lambda^m} \delta(\lambda) \right) \exp \left\{ i\lambda \left( \frac{4\pi N e^2}{\ell V} \sum_{\vec{k}} 1/k^2 \right) + A(\lambda) \right\} \\ &= V^{2N} \left[ i^m \frac{d^m}{d\lambda^m} \left\{ \exp \left( i\lambda \left( \frac{4\pi N e^2}{\ell V} \sum_{\vec{k}} 1/k^2 + A(\lambda) \right) \right) \right\} \right]_{\lambda=0} \end{aligned}$$

(A-8)

In particular,  $\langle \epsilon_0^0 \rangle = V^{2N}$ , and

$$\langle \epsilon_0^1 \rangle = 0, \quad (A-9)$$

$$\langle \varepsilon_o^2 \rangle = \frac{V^{2N}}{\pi} \left( \frac{Ne^2}{\ell} \right)^2 . \quad (A-10)$$

(These are the results needed in Sec. IV.)

By writing Eq. (A-7) in the form ( $\alpha^2 \equiv 4\pi Ne^2/\ell V$ )

$$\frac{\Omega(\varepsilon_o)}{V^{2N}} = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda(\varepsilon_o + \varepsilon_{\text{self}})} \prod_{\vec{k}} (1 + i\alpha^2 \lambda/k^2)^{-1} . \quad (A-11)$$

We can determine the way in which  $\Omega(\varepsilon_o)$  falls off at large  $\varepsilon_o$ .

( $\varepsilon_o + \varepsilon_{\text{self}}$  is never negative.) As  $\varepsilon_o \longrightarrow +\infty$ , we may push the contour of  $\lambda$  integration up in the complex plane and encounter an infinite sequence of (multiple) poles at  $\lambda = ik^2/\alpha^2$ . The closest ones of these are at  $|\vec{k}| = 2\pi/L$ , and give an asymptotic decay of  $\Omega(\varepsilon_o)$  as  $\mathcal{P}(\varepsilon_o) \exp \left[ -\varepsilon_o 4\pi^2/\alpha^2 L^2 \right]$ , as  $\varepsilon_o \longrightarrow \infty$ , where  $\mathcal{P}(\varepsilon_o)$  is a polynomial of degree at most equal to the multiplicity of the pole at  $\lambda = i(2\pi)^2/L^2 \alpha^2$ . For a range of  $\varepsilon_o > 0$  this means that Eq. (19) is normalizable directly, but above that range of  $\varepsilon_o$  we must use (18) to insure normalizability.

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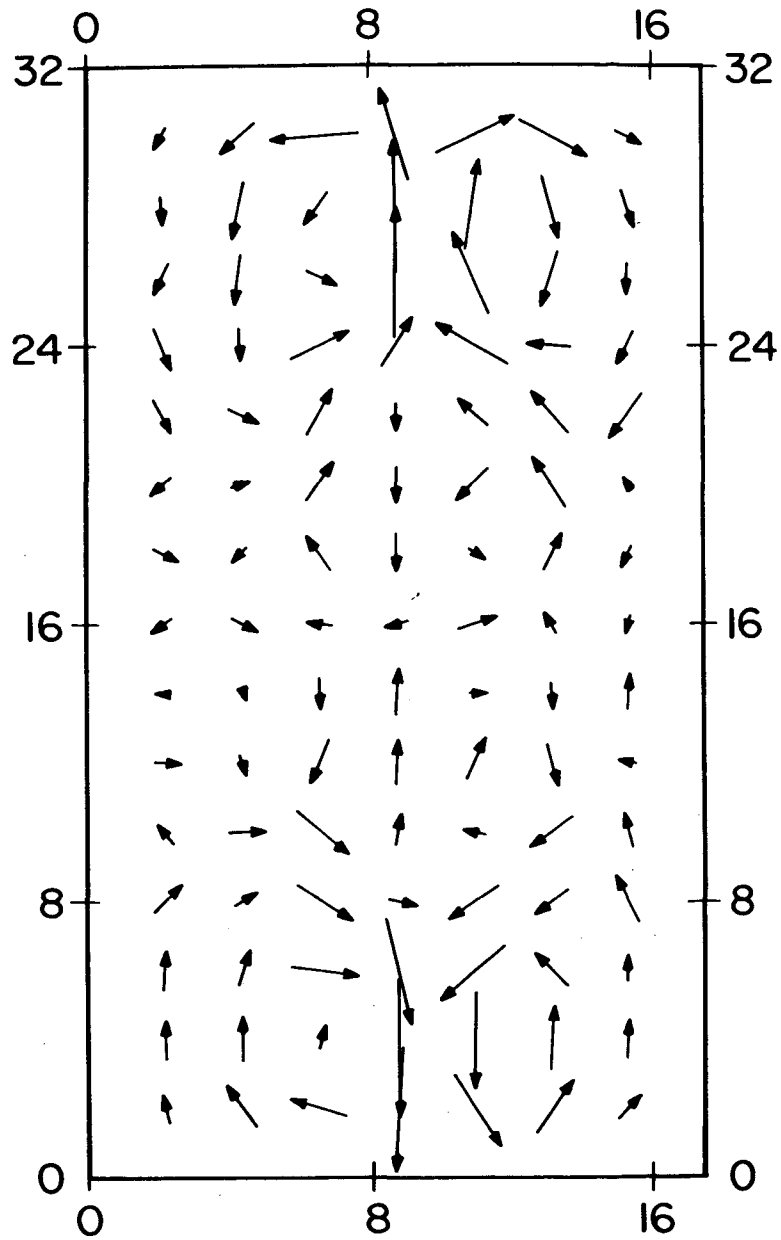
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## FIGURE CAPTIONS

Fig. 1 The fluid velocity vector field as a function of spatial position for the case of 4008 particles with interaction energy  $\cong 2.3$  times the self energy: (a) initially and (b) at  $t = 160.0$ . The velocity field at all later times is qualitatively similar to that at  $t = 160$ . The lengths of the arrows are normalized to  $V\text{-MAX}$ , the maximum dimensionless velocity present at any instant. This case should correspond to negative temperatures.

Fig. 2 The fluid velocity vector field as a function of spatial position for the case of 4008 particles with interaction energy  $\cong 0.43$  times the self energy: (a) initially and (b) at  $t = 375$ . The lengths of the arrows are normalized to  $V\text{-MAX}$ , the maximum dimensionless velocity present at any instant. This case should correspond to positive temperatures. The velocity field in (2b), which is similar at all later times, differs from that in (1b) by the absence of the two larger vortices.

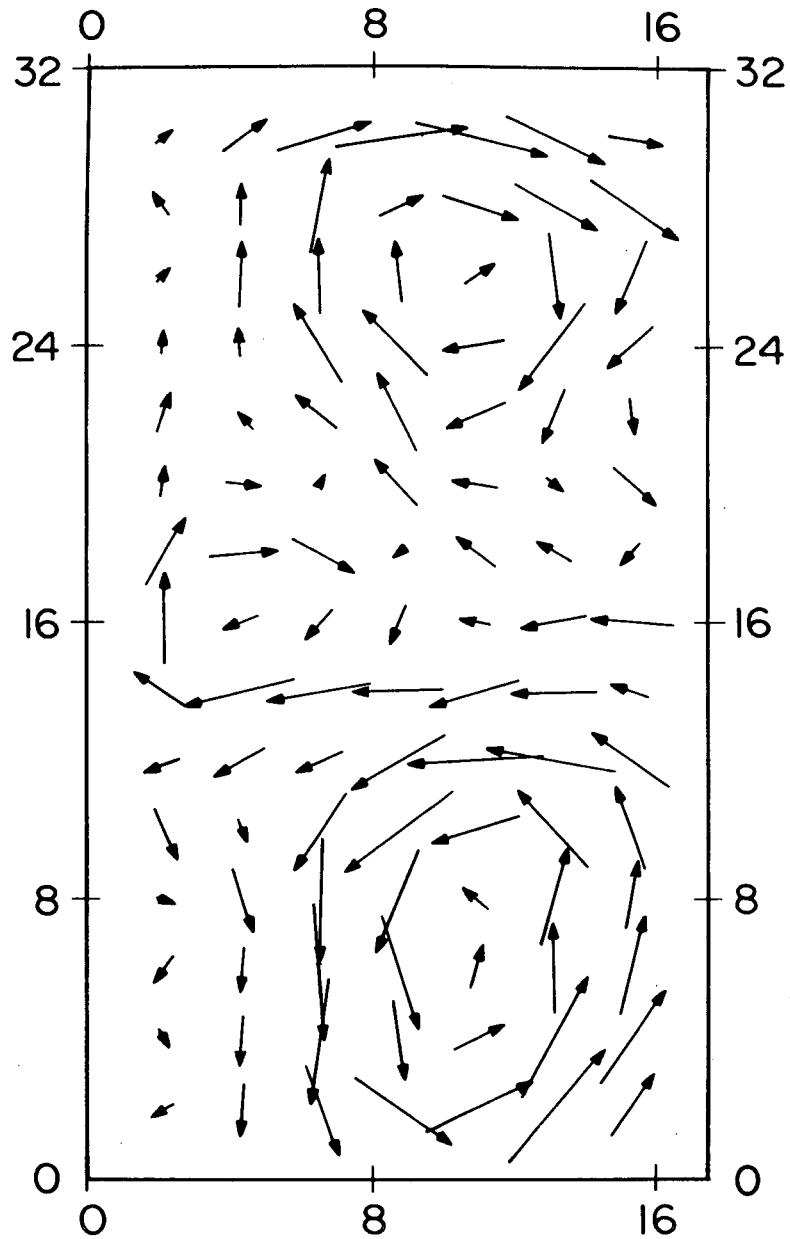
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TIME = 0.0  
V-MAX = 2.7845

Fig. 1a

B-673-156

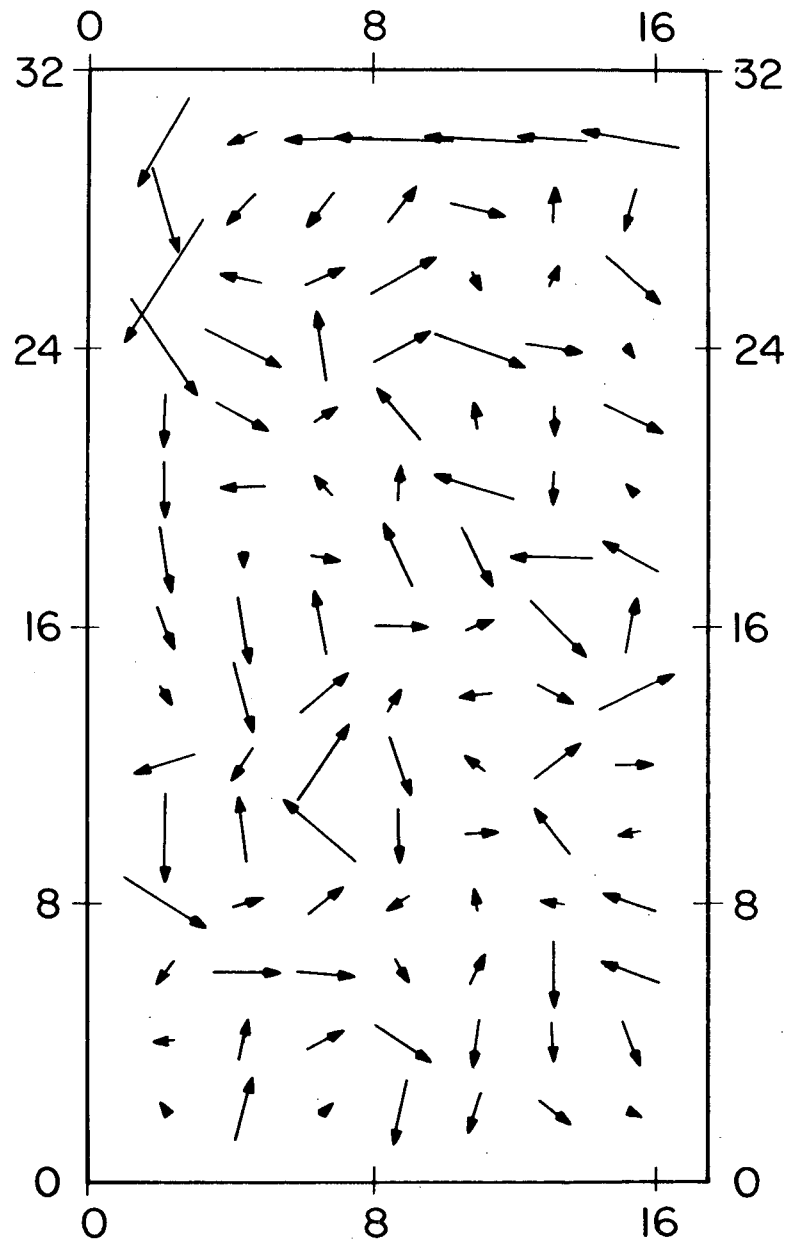


TIME = 160.0

V-MAX = 1.8794

Fig. 1b

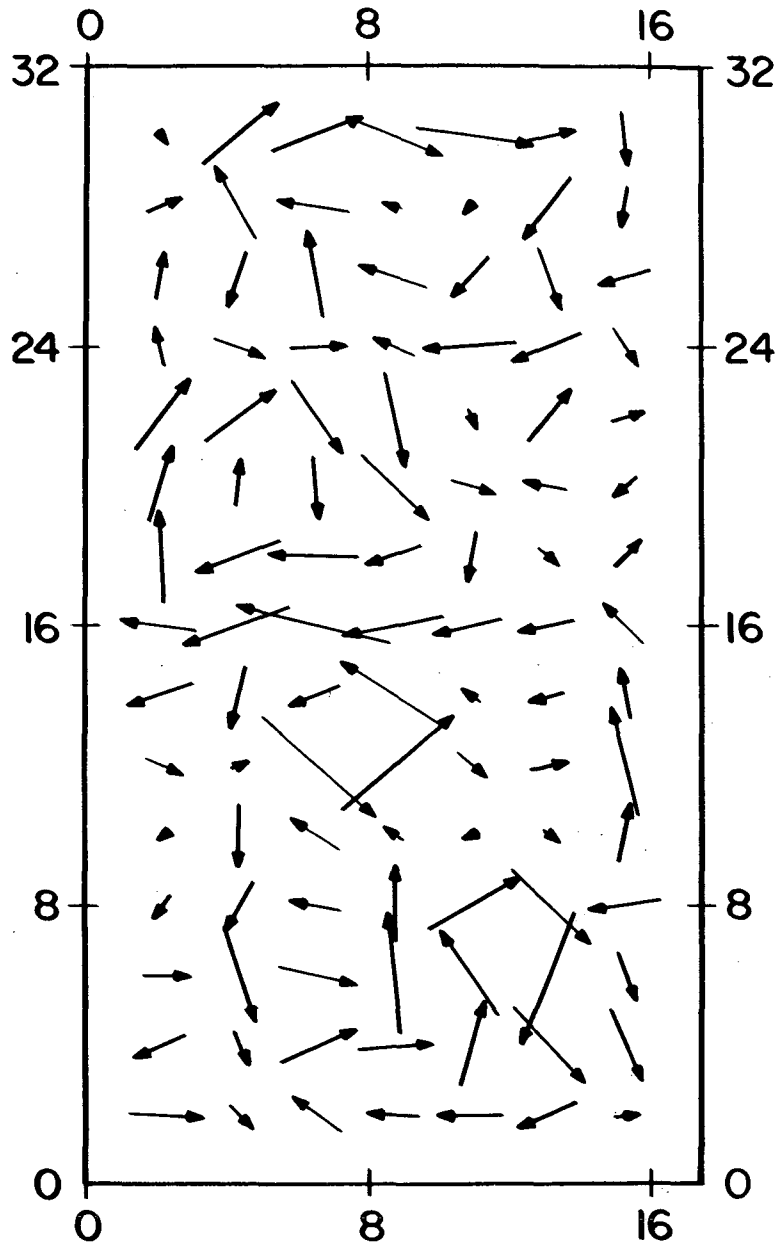
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TIME = 0.0  
V-MAX = 0.8307

Fig. 2a

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TIME = 375  
V-MAX = 0.7540

Fig. 2b